THE EXPLICIT JUMP IMMERSED INTERFACE METHOD AND INTEGRAL FORMULAS

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Abstract. Li and LeVeque's recent *Immersed Interface Method, SIAM J. Numer. Anal.,* **31***, 1994, pp. 1019—1044,* has been used on a multitude of problems ranging from Electrostatics to Traffic Flow. We give a summary of the different uses of the IIM, and proceed by connecting the IIM with analytic descriptions in the simplest cases.

The well known discretization of the Dirichlet boundary condition for the Laplace equation for grid–aligned boundaries is shown to be a special case of the Explicit Jump Immersed Interface Method. For one-dimensional boundary value problems, Schur–complements for finite difference discretizations are pointwise discretizations of integral formulas, and fast solvers may be viewed as efficient evaluation of integral formulas. The analogy requires a discretization of the delta and dipole, which may occur even on the domain boundary.

1. Introduction

The numerical treatment of interfaces and boundaries is very important as computers become powerful enough to deal with less idealized and more realistic problems. Free boundary value problems in general and more specifically design, control and inverse problems require the fast and automatic treatment of general geometries and boundary or interface conditions. The solution of any particular pde is merely a step toward the solution of the "real" problem, and should be solved as accurately and quickly as needed under this "stepping stone" view.

One approach to deal with these requirements, in particular the automation, is to use uniform meshes and deal with the boundaries and interfaces separately. Early examples are the Immersed Boundary Method (IBM), [18, 19, 23] and Mayo's treatment of the Poisson and Biharmonic equations in irregular regions [17]. [2] used Mayo's truncation error point of view to analyze Peskin's discrete delta approach. Motivated by this work, Li and LeVeque invented the Immersed Interface Method (IIM), [8], to treat the elliptic discontinuous variable coefficient ("interface") case. The IIM has since been used for several applications and extended in several directions, notably to hyperbolic and parabolic problems. The strong dependence of the error on the relative position of interface and grid for even moderate contrast in the coefficients (at least in the conductive case, [24]), and the lack of fast solvers, turned out to be slight problems suffered by the original IIM. In [8], the discontinuities were always "mild" in the sense that the contrast (quotient between limits of β on the sides of the interface) is always less than 10. Both of these limitations were obstacles for the use in inverse problems and for the extension of the discontinuous coefficient IIM to 3D, because fine grids were needed for good quality of solutions, and the problems would become enormous.

Li applied the IIM idea in his dissertation [11] to 3D (with an implementation for spherical interfaces; see also [12]), heat equations in 2D with fixed interfaces, Stokes flow with moving interfaces in 2D (see also [9]) and heat equations in 1D with moving interfaces. He also extended the IIM to the nonlinear case in [13] in a different fashion from our own work [28].

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A breakthrough occurred with the advent of Li's paper *A Fast Iterative Algorithm for Elliptic Interface Problems* [14]. We will refer to this method as the Fast Iterative IIM (FIIIM). Li used the observation that for piecewise constant coefficients, the equation can be written as a Poisson equation by dividing through the coefficient, if in addition one observes the jump conditions across the interface. This leads naturally to the idea of splitting the finite differences near the interface into the standard differences and **corrections** to the standard differences, and brings the FIIIM closer to the IIM for singular sources, Peskin's IBM and Mayo's approach. The jumps in the function and its derivatives (and not jumps like $[\beta u_n]$ as considered in [8]) turn out to be the crucial quantities. Given the jumps, the FIIIM was in the same situation as Mayo and Peskin: only corrections to the right hand side of the linear system are needed. Li chose to do this in the spirit of the original IIM, by selecting a point on the interface and developing Taylor expansions about it on both sides of the interface. The more difficult question was how to find the jumps. Lacking an integral equation as utilized by Mayo, Li used the equations for the jumps based on local properties of the solution derived in [8]. The jumps were computed only at the fixed set of control points and interpolated to intermediate points, and jumps in second derivatives were expressed as derivatives of jumps in the solution and first-order derivatives. In [27] it was observed that also jumps of higher than second order can always be expressed in terms of zeroth and first order discontinuities. This keeps the number of auxiliary unknowns low and fixed, even as the mesh is refined or when higher order methods are used.

Ultimately, a finer set of control points is needed to represent the interface more accurately, but for smooth interfaces fourth order interpolation by cubic splines allows the refinement of the control points to be much slower than the mesh refinement. The FIIM resulted in a linear system in the original unknowns (solution values on the grid) and auxiliary unknowns (jumps across the interface), with the standard five-point discretization of the Laplacian as the biggest of four blocks in the matrix. Eliminating the original unknowns results in a small, non-symmetric system for the auxiliary unknowns, a Schur complement, that can be solved quite efficiently with an iterative method (e.g. GMRES; see [21]). Each iteration requires the application of a fast Poisson solver on the rectangle, but only a few iterations are needed. A fast version of the IIM for piecewise constant coefficients was born! In addition, by making the coefficients of the corrections to the standard differences small (essentially significantly widening the original six-point stencil, and ensuring that coefficients decay in magnitude away from the diagonal by using a weighted least squares method), Li found a much more stable version of the IIM that does better than the IIM on large contrast problems both in the resistive and conductive case. The Schur–complement formulation is quite similar to earlier fast elliptic solvers on irregular domains, e.g. by Proskurowski and Widlund, [20]. In [27], a change of variables which was also used by Golub and Concus[5] yields a fast method for piecewise smooth coefficients.

Li went on to replace his original spline interface with a level set method, which allowed him to compute moving interface problems successfully even in the presence of changes in the topology of the interface with T. Y. Hou, H. Zhao and S. Osher [6], used this to study electron migration with H. Zhao and H. Gao [16], and Stefan Problems with B. Soni [15] The slow solvers for the original IIM were studied and improved by Adams with a multigrid approach [1]. Yang [29] extended the IIM "back" to Mayo's earlier problem on irregular domains and combined her IIM for Boundary Value Problems (IIMB) with the original IIM to treat fluid flow problems in complicated geometries with discontinuous permeabilities, using Adams' multigrid [1] as the fast solver for variable coefficient problems. Zhang [30] and LeVeque and Zhang [10] showed how to use the IIM for hyperbolic systems of partial differential equations with discontinuous coefficients arising from acoustic or elastic problems in heterogeneous media. The latter two uses of the IIM were successfully combined with LeVeque's CLAWPACK software package [7]. Calhoun [3] and Calhoun and

LeVeque [4] extended the IIM to a stream-function vorticity formulation of incompressible flow in 2D.

The Explicit Jump Immersed Interface Method (EJIIM, [27]) places the auxiliary variables at the intersection of the interface with the mesh like Mayo and uses one-sided interpolation to approximate the jump equations. This allows the same treatment for all three fundamental discontinuous elliptic problems. The non–differentiability may arise from singularly supported sources in the equation, from embedding the domain of interest in a larger domain, or from discontinuities in the coefficients of the differential equation (interfaces). In the remainder of this article we focus on elliptic equations with singular sources and on irregular regions, for other types of equations and the interface case we refer to [8] and [27] and the previously cited literature.

The FIIIM and EJIIM exploit fast solvers for constant coefficients on uniform Cartesian grids to also find fast solutions on irregular domains or for variable discontinuous coefficient problems. A fast solver for an elliptic differential equation can be viewed as approximating the integration against a singular kernel as required in a boundary integral approach [27], while allowing great flexibility in boundary conditions, body forces and the use as a preconditioner in inhomogeneous problems. The one-dimensional "Singular Poisson Equation" and one-dimensional Boundary Value Problems (BVP) are considered for two reasons. In 1D, the connections between the discretization of the differential equation (and its fast solver) and integral equation are exact while in higher dimensions insights from potential theory are required and the discretizations are only approximate. Secondly, the treatment of discontinuities in solutions and their derivatives is much simpler in 1D, because of the simple one-point structure of boundaries and interfaces. Except for these simplifications, the EJIIM is the same in higher dimensions.

We will illustrate several aspects of the EJIIM with simple examples.

1. *Integral equation interpretation of well-known discretization approaches.*
2. *Irregularity of the discrete solution of an elliptic differential equation.*
3. *Preconditioning a discretized differential equation by a fast solver and integral formulas.*
4. *Schur–complements and Boundary Integral formulas.*

To emphasize the introductory nature of this work, we have included remarks that encourage the readers to fill in details.

2. Poisson problem, Green's kernel and their discretizations

2.1. **A 1D Poisson problem.** Let f in $C^1(0,1)$. Consider the 1D Poisson problem

$$\begin{aligned} u_{xx} &= f, \\ u(0) &= 0, \\ u(1) &= 0. \end{aligned} \tag{1}$$

We integrate f, determine the two constants of integration and see that it is solved by

$$\begin{aligned} u(x) &= \int_0^x \int_0^y f(\xi) d\xi dy - x \int_0^1 \int_0^y f(\xi) d\xi dy \\ &= \int_0^x (x-y) f(y) dy - x \int_0^1 (1-y) f(y) dy \\ &= \int_0^x (x-y) f(y) dy - \int_0^x x(1-y) f(y) dy - \int_x^1 x(1-y) f(y) dy \\ &= \int_0^x (x-1) y f(y) dy + \int_x^1 (y-1) x f(y) dy \\ &= \int_0^1 G(x,y) f(y) dy, \text{ for } x \in [0,1]. \end{aligned} \tag{2}$$

Here, the *Green's kernel*[1] for the interval $[0,1]$ is

$$G(x,y) = \begin{cases} (x-1)\,y & 0 \le y \le x \le 1, \\ (y-1)\,x & 0 \le x \le y \le 1. \end{cases} \tag{3}$$

We view integration against the Green's kernel (3) as a global operation that solves the differential equation (1) with boundary conditions*by inverting the differential operator including boundary conditions*.

2.2. **The discrete 1D Poisson problem.** The usual centered finite differences

$$\frac{u_{i-1} - 2u_i + u_{i+1}}{h^2} = f_i \tag{4}$$

are used in the discretization of (1) on equidistant interior grid points $x_i = ih$, $i = 1, 2, \ldots, n-1$, with $h = 1/n$. When $u_{xx} = f$ is differentiable, the truncation error is seen via Taylor expansions to be

$$T_i = f(x_i) - \frac{u(x_{i-1}) - 2u(x_i) + u(x_{i+1})}{h^2} = O\big(h^2\big)\,. \tag{5}$$

For the two interior points next to the boundary, we use the boundary conditions $u(0) = u_0 = 0$ and $u(1) = u_1 = 0$ and find

$$\begin{aligned} u_{xx}(h) &= \frac{0 - 2u(h) + u(2h)}{h^2} + O\big(h^2\big)\,, \\ u_{xx}(1-h) &= \frac{u(1-2h) - 2u(1-h) + 0}{h^2} + O\big(h^2\big)\,. \end{aligned}$$

Writing (4) in matrix form, the Poisson problem is discretized as

$$\mathcal{A}U = F. \tag{6}$$

For example, on the grid with $h = 1/4$, i.e. on the points $\{0, 0.25, 0.5, 0.75, 1\}$, the differential operator ∂_{xx} including the boundary conditions $u(0) = u(1) = 0$ is discretized by the matrix

$$\mathcal{A}_3 = \frac{1}{h^2} \begin{pmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{pmatrix}$$

The entries in U approximate the solution at the interior points $\{0.25, 0.5, 0.75\}$ and $F = [f(0.25), f(0.5), f(0.75)]^T$ approximates the right hand side. In general, for Dirichlet boundary conditions, the discrete solution lives on the $n-1$ interior points of the discretization of $[0,1]$ by n intervals with $h = 1/n$. We will see in §4 that problems with non-vanishing Dirichlet boundary data are numerically approximated *by the same matrix* $\mathcal{A}$ as Poisson problems, but with singular right hand side.

2.3. **Connection between the discretization of the differential equation and the integral formula.** The matrix $\mathcal{A}$ is tridiagonal, and U can be found in $\mathcal{O}(n)$ operations. In higher dimensions, this is not the case and we turn to fast solvers in Fourier space (Fast Poisson solvers, [26]) instead. From [27] we know

Lemma 1. *The (i,j) entry of* $\mathcal{A}^{-1} \in \mathbf{R}^{(n-1)\times(n-1)}$ *(for* $n > 3$*) is*

$$a_{ij} = \frac{\min(i,j)\,(\max(i,j) - n)}{n^3}.$$

[1] This is an unfortunate misnomer because it really is the kernel for the Poisson problem, and should be called Poisson kernel — but this name is reserved for the kernel for the Dirichlet problem!

For the above example this gives

$$\mathcal{A}^{-1} = -\frac{1}{64}\begin{pmatrix} 3 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 3 \end{pmatrix}.$$

Also from [27], we know that

Lemma 2. *$\|\mathcal{A}^{-1}\|_\infty = \frac{1}{8}$ for n even and $\|\mathcal{A}^{-1}\|_\infty = \frac{1-n^{-2}}{8}$ for n odd.*

This uniform boundedness of the inverse operator, together with the second order consistency of the discretization, combine to give second order convergence. The solution of the discrete problem is

$$U = \mathcal{A}^{-1}F, \tag{7}$$

The evaluation of the true solution on the grid points (denoted by Eu) satisfies

$$Eu = \mathcal{A}^{-1}(F - T). \tag{8}$$

where the norm of the truncation error is $\|T\|_\infty = O\big(h^2\big)$. Hence $\|U - Eu\|_\infty = \|\mathcal{A}^{-1}T\|_\infty \leq \|\mathcal{A}^{-1}\|_\infty \|T\|_\infty = O\big(h^2\big)$, and we have proved the following theorem.

Theorem 3. *As the grid is refined, the solution of the discretized problem converges in the infinity norm on grid points with second order to the solution of the differential equation.*

The main point of this § is the analogy between (7) and (2). The entries of $\mathcal{A}^{-1}$ in (1) are equal to values of the Green's kernel (3) at the grid points, multiplied by h; this factor h corresponds to *integration* against the kernel. Instead of viewing (6) as discretizing the differential equation (1), we view the system (7) as discretizing the Green's kernel-based integral formula (2). Finite difference operators discretize differential operators including boundary conditions, and their inverses may approximate integral formulas!

3. Known discontinuities in the solution of a Poisson Equation

3.1. **Differential equations with singular sources.** Since the EJIIM deals with discontinuities in solutions of differential equations (or discontinuities in their derivatives), it is essential to have a good understanding of the *delta* and *dipole* (also called *doublet*). These distributions introduce irregularity into the solution of the Poisson equation when placed on the right hand side.

Definition 1 (1D delta, dipole)**.** *Let $\gamma \in (0, 1)$.*
The **delta** *$\delta(x - \gamma)$ (centered at γ) is the distribution that satisfies $\int_0^1 \Phi(x)\delta(x-\gamma)dx = \Phi(\gamma)$ for any function $\Phi \in C^\infty([0, 1])$.*
The **dipole** *$\delta'(x-\gamma)$ (centered at γ) is the distribution that satisfies $\int_0^1 \Phi(x)\delta'(x-\gamma)dx = -\Phi'(\gamma)$ for any function $\Phi \in C^\infty([0, 1])$.*

Definition 1 gives mathematically precise meaning, while the following aspects are also important for understanding EJIIM.

1. *The delta and dipole are convenient short notation for the fact that a solution of a differential equation has a discontinuous derivative, or is discontinuous itself.* This view will allow us to apply the standard "integration against a kernel" approach to find solutions of the differential equation.
2. *The delta and dipole can be viewed as "singular" limits of certain C^∞ functions with fixed L^1 norm as their support vanishes.* This view helps interpret our discretization of the differential equation.
3. *The delta and dipole are useful for making sense of* integration by parts*, an essential tool for differential equations.* This view will initially be least useful for EJIIM, but is the most easily appreciated interpretation. Later, we will see a correspondence between integration by parts (Green's identities) on the differential equation side and Schur complements on the discretized equation side.

An immediate benefit of introducing the delta is the characterization of the Green's kernel in a form that carries over to higher dimensions. The importance of the formula (2) for the solution of the Poisson problem lies in the fact that it is valid even for singular (distributional) right hand side f and that ot carries over verbatim to higher dimensional Poisson problems, at least for sufficiently nice domains. In 1D, the Green's kernel satisfies $\partial^2 G(x,y)/\partial x^2 = \delta(x-y)$ with $G(0,y) = G(1,y) = 0$ for all $y \in (0,1)$. It is symmetric and negative everywhere in $(0,1)\times(0,1)$. In higher dimensions, too, there exists a unique G defined by just the above properties: It satisfies a Poisson equation with a delta on the right hand side, vanishes on the boundaries, is symmetric in x and y, and is negative where finite.

Consider the integral formula (2) for the Poisson problem with the following four increasingly singular right hand sides. The irregularity occurs always at the same point $\alpha \in (0,1)$; by 1_Ω we mean the characteristic function of the set Ω.

1. $f = (x-\alpha)1_{\{\alpha<x<1\}}$ (f continuous but not differentiable)
2. $f = 1_{\{\alpha<x<1\}}$ (f discontinuous)
3. $f = \delta(x-\alpha)$ (f first order singular)
4. $f = \delta'(x-\alpha)$ (f second order singular)

For all 4 cases, the solution via (2) makes sense. The reader is asked to convince herself in Remark 3.3 that these solutions satisfy the differential equation in the classical sense away from α, while becoming more and more singular at α. Technically, G does not satisfy the requirements on the test function Φ in the definitions of the delta and dipole. The biggest problem occurs in applying the dipole at the kink of G, where the derivative does not exist. However, for any $u(\alpha)$ the solution

$$u(x) = \int_0^1 G(x,y)\delta'(y-\alpha)dy = -\frac{\partial G}{\partial y}(x,\alpha) = \begin{cases} -x & x<\alpha, \\ u(\alpha) & x=\alpha, \\ 1-x & \alpha<x, \end{cases}$$

is conceivable, with $u(\alpha) = 1/2-\alpha$ most satisfactory because it it has the property that values of u are the averages of one-sided limits. For continuous f, we find that $u \in C^2$; for discontinuous f, we get $u \in C^1$; for first order singular f, we get $u \in C^0$ and for second order singular f, we get $u \in H^1$, the subspace of functions in L^2 whose derivative is also in L^2. In all cases, only one of the derivatives of u is discontinuous[2], and the magnitude of the jump[3] is 1.

Remark 3.1. *In one space dimension, the Green's kernel is* $G(x,y) = N(y-x)+H(x,y)$, *where* N *is the fundamental solution (Newtonian potential) that satisfies* $\Delta N = \delta(x)$ *and* H *is a harmonic (in 1D, that means affine) function in* x *for every* y *which is introduced to achieve the desired boundary values:* $H(0,y) = -N(y)$ *and* $H(1,y) = -N(y-1)$. *Usually the fundamental solution is made unique by specifying its asymptotic behavior near infinity. For the (nonstandard)* N *in 1D, we require* $\inf(N) = 0$.

3.2. **EJIIM for singular sources.** The conceptually easiest application of EJIIM is the numerical approximation of problems with right hand sides of the type 1-4. This is the context in which Li and LeVeque's Immersed Interface Method [8, 11] is preceded by Peskin's Immersed Boundary Method [18] and Mayo's Fast Poisson solvers on irregular domains [17]. The EJIIM formulas from [27] deal with two issues at the same time:

1. The truncation error in (4) deteriorates as u becomes less smooth.
2. We need to discretize singular f.

The idea is to use the knowledge of the irregularity of u introduced by f (as given by the integral formula) and to build it into the discretization. The strength of the dipole is

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[2] By convention, u is its own zeroth derivative.

[3] From a practical point of view, the search for non-smooth solutions of the differential equation with prescribed jumps is the reason to study singular f.

the jump in u, the strength of the delta is the jump in u_x, the jump in f is the jump in u_{xx}, the jump in f_x is the jump in u_{xxx} and so forth. This results simply in "corrections" to the standard formulas applicable on the right hand side of the discretization (4) for the smooth case; these corrections may be viewed as a discretization of the singularity of f. Contributions of different singularity are each separated into the strength of the discontinuity and the discretization of the normalized singularity, i.e. how it influences the solution on the grid.

In this sense we will speak of grid functions resulting from discretizations of second order differential equation as "differentiable", "not differentiable" and "discontinuous" between grid points if the right hand side for the two neighboring grid points behaves under refinement like $\mathcal{O}(1))$ (i.e. is a function), $\mathcal{O}(h^{-1}))$ (i.e. is first order singular) and $\mathcal{O}(h^{-2}))$ (i.e. is second order singular), respectively.

We copy the main result on how to do this from [27] as Lemma 4. Square brackets $[u^{(m)}] = u^{(m)}(\alpha^+) - u^{(m)}(\alpha^-)$ indicate jumps, i.e. the difference subtracing the left limit of u at the point α from the right limit.

Lemma 4 (jump-corrected differences)**.** *Let $x_j \leq \alpha < x_{j+1}$, $h^- = x_j - \alpha$ and $h^+ = x_{j+1} - \alpha$. Suppose $u \in C^4[x_j - h, \alpha) \cap C^4(\alpha, x_{j+1} + h]$, with derivatives extending continuously up to the boundary α. Then the following approximations hold to $O(h^2)$:*

$$u_x(x_j) \approx \frac{u(x_{j+1}) - u(x_{j-1})}{2h} - \frac{1}{2h}\sum_{m=0}^{2}\frac{(h^+)^m}{m!}[u^{(m)}],$$

$$u_x(x_{j+1}) \approx \frac{u(x_{j+2}) - u(x_j)}{2h} - \frac{1}{2h}\sum_{m=0}^{2}\frac{(h^-)^m}{m!}[u^{(m)}],$$

$$u_{xx}(x_j) \approx \frac{u(x_{j+1}) - 2u(x_j) + u(x_{j-1})}{h^2} - \frac{1}{h^2}\sum_{m=0}^{3}\frac{(h^+)^m}{m!}[u^{(m)}], \tag{9}$$

$$u_{xx}(x_{j+1}) \approx \frac{u(x_{j+2}) - 2u(x_{j+1}) + u(x_j)}{h^2} + \frac{1}{h^2}\sum_{m=0}^{3}\frac{(h^-)^m}{m!}[u^{(m)}]. \tag{10}$$

The system (6) becomes

$$\mathcal{A}U = F + \Psi C \tag{11}$$

where $C \in \mathbf{R}^4$ is the vector of jump strengths $\{[u], [u_x], [u_{xx}], [u_{xxx}]\}$as in Lemma 4, and $\Psi \in \mathbf{R}^{n-1} \times \mathbf{R}^4$ has two non-zero entries per column, introducing the jumps in C into the j^{th} and $(j+1)^{st}$ equations with the correct geometry. For example the first column corresponds to $[u]$ and has non-zero entries $\Psi(1, j) = 1/h^2$ and $\Psi(1, j+1) = -1/h^2$. In Remark 3.4 the reader is asked to convince herself that Theorem 3 still holds for this singular case and even if the corrections are used only up to $[u_{xx}]$.

Remark 3.2. *Plotting $\Psi(1, \cdot)$ and $\Psi(2, \cdot)$ for fixed α, $x_j \leq \alpha < x_{j+1}$, as $n \to \infty$ gives geometric intuition of the discrete dipole $\Psi(1, \cdot)$ and the discrete delta $\Psi(2, \cdot)$.*

Remark 3.3. *a) The solutions of problem (1) with f given by*

1. $f_1 = (x - \alpha)1_{\{\alpha < x < 1\}}$,
2. $f_2 = 1_{\{\alpha < x < 1\}}$,
3. $f_3 = \delta(x - \alpha)$,
4. $f_4 = \delta'(x - \alpha)$.

are

$$u_1(x) = \begin{cases} a_1 x, & 0 \le x < \alpha \\ a_1 x + (x-\alpha)^3/6, & \alpha < x \le 1 \end{cases}, \quad \textit{where } a_1 = -(1-\alpha)^3/6,$$

$$u_2(x) = \begin{cases} a_1 x, & 0 \le x < \alpha \\ a_1 x + (x-\alpha)^2/2, & \alpha < x \le 1 \end{cases}, \quad \textit{where } a_1 = -(1-\alpha)^2/2,$$

$$u_3(x) = \begin{cases} (\alpha-1)x, & 0 \le x < \alpha, \\ (x-1)\alpha, & \alpha < x \le 1, \end{cases}$$

$$u_4(x) = \begin{cases} -x, & 0 \le x < \alpha, \\ 1-x, & \alpha < x \le 1. \end{cases}$$

b) Knowledge of the jumps in u and jumps in its derivatives and discretization via Lemma 4 leads to a pointwise recovery of the solutions from part a) for any uniform mesh.

Remark 3.4. *a) Given right hand side f that is smooth except for singularities up to second order at a finite number of points and using (9) and (10), the discrete solutions of (1) converges to the solution of the continuum problem like $O(h^2)$ in the maximum norm on grid points. b) The result in a) holds even if the $[u_{xxx}]$ terms are dropped from (9) and (10). The fundamental idea is that the discretized integration against the kernel smoothes the only locally large truncation error by one order.*

4. Dirichlet BVP via Poisson Problem

4.1. **A 1D Dirichlet problem.** Let u_0 and $u_1 \in \mathbf{R}$, and consider the Dirichlet BVP:

$$u_{xx} = 0 \quad \text{in } (0,1), \tag{12}$$

$$u(0) = \bar{u}_0, \tag{13}$$

$$u(\alpha) = \bar{u}_1. \tag{14}$$

First consider the case $\alpha = 1$. Existence and uniqueness of the solution of this problem are trivial,

$$u(x) = \bar{u}_0 + x\,(\bar{u}_1 - \bar{u}_0), \text{ for } x \in [0,1]. \tag{15}$$

There exists another important way to write the solution, which is analoguous to standard boundary integral methods in higher dimensions:

$$u(x) = -\frac{\partial}{\partial y} G(x,y)\Big|_{y=0} \bar{u}_0 + \frac{\partial}{\partial y} G(x,y)\Big|_{y=1} \bar{u}_1. \tag{16}$$

The kernel here, *the outward normal derivative of the Green's kernel along the boundary*, is known as the *Poisson kernel* in higher dimensions. We need to interpret (16) for $x = 0$ and $x = 1$, because in these cases the derivatives at $y = 0$ and $y = 1$, respectively, do not exist. However, both one sided limits for the derivatives of G exist in both cases, and taking the limits for $y \in (0,1)$ yields exactly (15), while applying the limits for $y \notin (0,1)$ results in $u(0) = u(1) = 0$.

We choose to write the solution in the following peculiar form, using the solution for a *Poisson problem* by integration against the Green's kernel (2) to solve a *Dirichlet problem*!

$$u(x) = \lim_{\epsilon \to 0+} \int_0^1 G(x,y)\left(u_0 \delta'(y-\epsilon) - u_1 \delta'(y-(1-\epsilon))\right) dy = \tag{17}$$

$$= \lim_{\epsilon \to 0+} \int_0^1 G(x,y)\left([u]_0 \delta'(y-\epsilon) + [u]_1 \delta'(y-(1-\epsilon))\right) dy, \text{ for } x \in (0,1).$$

The sole purpose of the limit in this formula is to define the application of δ' to G at a point of discontinuity by using a one-sided limit. On the boundary, i.e. for $x \in \{0,1\}$, (17)

does not agree with (15). The function defined by (17) on $[0,1]$ has jumps $[u]_0 = u_0$ and $[u]_1 = -u_1$ at the left and right endpoints, respectively!

4.2. **The discrete 1D Dirichlet problem.** Consider again $n = 4$, discretize the differential operator on interior points as for the Poisson problem, and the boundary condition at the boundary points.

$$\frac{1}{h^2}\begin{pmatrix}1 & 0 & 0 & 0 & 0\\ 1 & -2 & 1 & 0 & 0\\ 0 & 1 & -2 & 1 & 0\\ 0 & 0 & 1 & -2 & 1\\ 0 & 0 & 0 & 0 & 1\end{pmatrix}\begin{pmatrix}u_0\\ u_1\\ u_2\\ u_3\\ u_4\end{pmatrix} = \begin{pmatrix}\bar{u}_0/h^2\\ 0\\ 0\\ 0\\ \bar{u}_1/h^2\end{pmatrix} \tag{18}$$

Elimintion of known variables is the easiest example of a Schur–complement and yields

$$\mathcal{A}_3 U = \left(-\frac{1}{h^2}\begin{pmatrix}\bar{u}_0\\ 0\\ \bar{u}_1\end{pmatrix}\right). \tag{19}$$

The solution of our discrete model problem on $\{0, 0.25, 0.5, 0.75, 1\}$ is

$$U = \mathcal{A}_3^{-1}\left(-\frac{1}{h^2}\begin{pmatrix}\bar{u}_0\\ 0\\ \bar{u}_1\end{pmatrix}\right) = \mathcal{A}_3^{-1}\begin{pmatrix}-\left[u\right]_0/h^2\\ 0\\ \left[u\right]_1/h^2\end{pmatrix}, \tag{20}$$

which results from simply moving the known boundary values in the discretization of the Laplacian (4) onto the right hand side. The standard way of solving the Dirichlet problem (20) discretizes (17) just as (7) discretizes (2). Also, (20) is a special case of (9) and (10) in the following sense:

Consider $x_{n-1} \leq \alpha < 1$, and recall that the discretization of the Poisson problem $\mathcal{A}$ imposes $u(1) = 0$ on the discretization. Equation (9) in this case is

$$u_{xx}(x_{n-1}) \approx \frac{0 - 2u(x_{n-1}) + u(x_{n-2})}{h^2} - \frac{1}{h^2}\sum_{m=0}^{3}\frac{(1-\alpha)^m}{m!}[u^{(m)}]_1. \tag{21}$$

In the limit as $\alpha \longrightarrow 1$, this becomes

$$\begin{aligned} u_{xx}(x_{n-1}) &\approx \frac{-2u(x_{n-1}) + u(x_{n-2})}{h^2} - \frac{1}{h^2}\sum_{m=0}^{3}\frac{0^m}{m!}[u^{(m)}]_1 = \\ &= \frac{-2u(x_{n-1}) + u(x_{n-2})}{h^2} - \frac{[u]_1}{h^2}. \end{aligned}$$

So $u_{xx}(x_{n-1}) = 0$ and $u(1) = 0$ becomes

$$\frac{-2u_{n-1} + u_{n-2}}{h^2} = \frac{[u]_1}{h^2}$$

just as in (20). The question now becomes: What is the continuous equation discretized by (4), modified to (21) at x_{n-1}?

4.3. **Connection between the discretization of the differential equation and an integral formula.** The answer depends on what we use for $[u_x]$, $[u_{xx}]$ and $[u_{xxx}]$. For example, $[u_{xx}] = [f]$ and $[u_{xxx}] = [f_x]$ depend on the extension of f to $(\alpha, 1)$. For $f = 0$ on$(0, \alpha)$ the extensio is zero, and $[u_{xx}] = [u_{xxx}] = 0$; but in any case, $[u_{xx}]$ and $[u_{xxx}]$ can be known from the problem data. The choice of $[u_x]$ has a bigger impact. For EJIIM, we propose $[u_x] = -u_x^-$, while the earlier capacitance matrix approach [20] as incorporated into the IIM [29] used $[u_x] = 0$. In the first case, $[u_x]$ needs to be determined as part of the solution; in the second case, $[u_x]$ is known. This seeming disadvantage of the EJIIM is outweighed by the fact that for this choice of $[u_x]$ together with always extending f by 0 on $(\alpha, 1)$, the extension of u by zero $(\alpha, 1)$ satisfies all jump conditions and boundary conditions as well as the extension of the differential equation, and is the unique solution of

$u_x(\alpha) = 0$, $u(1) = 0$, $u_{xx}(x) = 0$ in $(\alpha, 1)$, where the first boundary condition follows from $[u_x] = u_x^- \Rightarrow u_x^+ = 0$. Finally, $u \equiv 0$ on $(\alpha, 1)$ and $[u]_\alpha = -\bar{u}_1$ guarantees $u^-(\alpha) = \bar{u}_1$. In the capacitance matrix approach, the correct boundary limit $u(1)$ needs to be found and f needs to be extended differentiably in order to make $u^+(\alpha) = 0$.

By D^T_{x,α^-} we denote the unique linear operator that extrapolates the derivatives of a grid function at α, based on the three grid points to the left of α, to second order. The EJIIM for (12)–(14) can be written as

$$\mathcal{A}U = \frac{1}{h^2}\begin{pmatrix} -[u]_0 \\ 0 \\ \\ \vdots \\ 0 \end{pmatrix} + \frac{(1-\alpha)}{h^2}\begin{pmatrix} 0 \\ \vdots \\ 0 \\ C \end{pmatrix},$$
$$C = -D^T_{x,\alpha^-}U.$$

Shortening D^T_{x,α^-} to D^T and writing $\tilde{F} = (-[u]_0, 0, \dots, 0)/h^2$ and $\Psi_1 = \left(0, 0, \dots, (1-\alpha)/h^2\right)^T$, this is

$$\mathcal{A}U = \tilde{F} + \Psi_1 C,$$
$$C = -D^T U.$$

The first set of equations includes (18)! We rewrite it:

$$U = \mathcal{A}^{-1}(\tilde{F} + \Psi_1 C),$$

and form the Schur complements for the variables U and C:

$$(I + \mathcal{A}^{-1}\Psi_1 D^T)U = \mathcal{A}^{-1}\tilde{F}, \tag{22}$$
$$(I + D^T\mathcal{A}^{-1}\Psi_1)C = -D^T\mathcal{A}^{-1}\tilde{F}. \tag{23}$$

Equations (22) and (23) are discretizations of the two integral equations that appear in the following Lemma.

Lemma 5. *The solution of the problem (12)–(14) and the jump $c = [u_x] = -u_x^-(\alpha)$ satisfy*

$$u(x) + \int_0^1 G(x,y)\delta(y-\alpha)\frac{d}{dx}u(x)\Big|_{x=\alpha^-} dy = \int_0^1 G(x,y)\left\{\delta'(y-\alpha)u_1 + \delta'(y-0)u_0\right\} dy, \tag{24}$$

$$c + \frac{d}{dx}\int_0^1 G(x,y)\delta(y-\alpha)c\, dy\Big|_{x=\alpha^-} = -\frac{d}{dx}\int_0^1 G(x,y)\left\{\delta'(y-\alpha)u_1 + \delta'(y-0)u_0\right\} dy\Big|_{x=\alpha^-}. \tag{25}$$

Proof. (25) follows immediately from (24) by applying $\frac{d}{dx}(\cdot)\big|_{x=\alpha^-}$ to both sides and renaming $c = \frac{d}{dx}(u)\big|_{x=\alpha^-}$, just as in the discrete case. To see that u must satisfy (24), we decompose $u = u_0 + [u_x]u_1 + [u]u_2$, where

$$\begin{array}{rclcrclrcl} \Delta u_0 &=& 0 & \text{with} & u_0(0) &=& \bar{u}_0, & u_0(1) &=& 0, \\ \Delta u_1 &=& \delta(x-\alpha) & \text{with} & u_1(0) &=& 0, & u_1(1) &=& 0, \\ \Delta u_2 &=& -\delta(x-\alpha) & \text{with} & u_2(0) &=& 0, & u_2(1) &=& 0, \end{array}$$

satisfy

$$u_0(x) = \int_0^1 G(x,y)(-\bar{u}_0)\delta'(y-0)dy = \begin{cases} 0 & x = 0, \\ \bar{u}_0(x-1) & 0 < x \le 1, \end{cases}$$
$$u_1(x) = \int_0^1 G(x,y)\delta(y-\alpha)dy = \begin{cases} (\alpha-1)x & 0 \le x < \alpha, \\ (x-1)\alpha & \alpha < x \le 1, \end{cases}$$
$$u_2(x) = -\int_0^1 G(x,y)\delta'(y-\alpha)dy = \begin{cases} -x & 0 \le x < \alpha, \\ 1-x & \alpha < x \le 1. \end{cases}$$

Adding the solutions,

$$u(x) = \int_0^1 G(x,y) \left\{ -\bar{u}_0 \delta'(y-0) + [u_x]\delta(y-\alpha) + \bar{u}_1 \delta'(y-\alpha) \right\} dy,$$

and moving unknown terms to the left (with $[u_x] = -u_x^-$) results in (24). □

Remark 4.1. *The Schur-complement (22) shows how preconditioning (presumably $\mathcal{A}^{-1}$ can be applied in a fast manner) can also correspond to transforming a differential equation into an integral equation, here (24). The Schur-complement (23) shows how algebraic manipulations on the discrete system (applying $-D^T$) can correspond to transforming an integral formula into a boundary integral formula, here (25).*

Remark 4.2. *The biggest difference between the grid–aligned boundary case and the unaligned boundary case is the introduction of the new discrete variable C, an unknown jump. In higher dimensions, this means many jumps, their number "proportional" to the length of the boundary. However, using a fast solver for the regular problem and the Schur–complement (23), we see that we have discretized a Fredholm equation of the second kind on the boundary (25), which is well known to behave nicely numerically. This observation has borne out in numerical studies, see* [27] *etc.*

Remark 4.3. *There exists an analogue of Lemma 1 for the case that (12) is replaced by $u_{xx} = f$ in (0,1).*

4.4. **Further examples of singular sources.** In [26], Laplace's equations and the 2D linear elastostatic equations are solved quickly on the rectangle with various boundary conditions, by reflecting the solution in each dimension and solving periodic problems on the larger domains. There nonzero boundary conditions on the original rectangle enter as singular sources in the equation on the extended domains.

4.5. **Comments on jump relations.** One of the major steps of the EJIIM is the derivation of (one-sided) jump relations. We have seen that for Laplace's equation, $[u], [u_x]$ and the problem data $([f], [f_x], \dots)$ is all we need. In 2D, this is also true as was shown in [27]. The idea in 2D is to take tangential derivatives on lower jumps and normal derivatives on the data, which we believe will extend to 3D without difficulties. In 3D, Schwab and Wendland [22] have developed integral equations for just these jumps, based on the same ideas. The advantage of EJIIM over true boundary integral methods lies in its ability to deal with body forces and extendibility to variable coefficients; the drawback is that for problems where boundary integral methods apply, they are probably faster than EJIIM (for fixed quality of solution).

5. Conclusions

We have explained the relationship between a finite difference discretization of the Laplacian and Green's kernels. The usual discretization of Dirichlet boundary values at grid points was shown to be a special case of the EJIIM, and fast Poisson–solver based Schur–complements were shown to discretize integral formulas. These connections serve to explain the EJIIM also in higher dimensions.

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